AD

AD-E402 413

Technical Report ARAED-TR-92038

INTERIOR BALLISTIC CALCULATIONS USING AN ACCURATE EQUATION OF STATE FOR THE PROPELLANT GASES

A.K. Macpherson
Lehigh University
Bethlehem, PA 18015

T. Vladimiroff
ARDEC

April 1993

U.S. ARMY ARMAMENT RESEARCH, DEVELOPMENT AND ENGINEERING CENTER

Armament Engineering Directorate

Picatinny Arsenal, New Jersey

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)

2. REPORT DATE
April 1993

3. REPORT TYPE AND DATES COVERED

4. TITLE AND SUBTITLE
INTERIOR BALLISTIC CALCULATIONS USING AN ACCURATE EQUATION OF STATE FOR THE PROPELLANT GASES

5. FUNDING NUMBERS

6. AUTHOR(S)
T. Vladimiroff, ARDEC
A.K. Macpherson, Lehigh University, Bethlehem, PA 18015

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESSES(S)
ARDEC, AED
Energetics and Warheads Div (SMCAR-AEE-BR)
Picatinny Arsenal, NJ 07806-5000

8. PERFORMING ORGANIZATION REPORT NUMBER
Technical Report
ARAED-TR-92033

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(S)
ARDEC, IMD
STINFO Br (SMCAR-IMI-I)
Picatinny Arsenal, NJ 07806-5000

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

The use of an accurate equation of state for propellant gases in interior ballistic calculations is very important for two reasons. The burning rate of the propellant depends on the pressure and it is the pressure that performs work on the projectile. Also, as interior ballistic codes become more sophisticated, propellant gas transport properties will have to be taken into account. Both viscosity and thermal conductivity should be important. Since different propellant gases have different transport properties, the composition of the propellant gas will have to be known as a function of time. It was shown many years ago that the Abel-Nobel equation, which is used for interior ballistic calculations is not very accurate. Also the covolume for each individual propellant is required thus introducing an extra adjustable parameter. In this work the interior ballistic code IBHVG2 is modified so that for each step of the ballistic cycle the equilibrium gas composition and pressure are calculated. The energy losses calculated by IBHVG2 are subtracted from the heat of formation of the propellant consumed before the equilibrium calculation is performed. The accurate equation of state proposed by Powell, Wilmot, Haar, and Klein is used. The covolume for each individual propellant is no longer required and the propellant gas composition inside the gun is monitored as a function of time. Ballistic performance using this approach is compared to the more conventional IBHVG2 calculation.

14. SUBJECT TERMS
Interior ballistics; Equation of state; MCVECE thermochemical code

15. NUMBER OF PAGES
16

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	SAR

CONTENTS

TABLES

INTRODUCTION

Computer modeling for the purpose of engineering design is becoming increasingly popular. This is mostly because computations can be performed much faster than the more conventional design cycle where a prototype is built and tested, the test results analyzed and a new prototype is built and tested until a final design is produced which passes all the required tests. The availability of powerful work stations at a reasonable cost can only be expected to accelerate this trend. The approach works well for mechanical parts where finite element analysis can be used to predict the stresses inside a material. For the design of propelling charges for large caliber guns the computational approach is less universally applied. This is probably because the interior ballistic event is quite complex. Propellant combustion and hydrodynamics must be modeled in great detail to be useful to the charge designer. Nevertheless, progress is being made and as the models become more accurate and the computers become faster, propelling charges will be designed mainly by computer.

It is obvious that as the models become more accurate they can provide more detailed predictions about the performance of a proposed charge design in the gun environment. It is always possible to produce a model which has adjustable parameters built in which can then be fixed in such a way as to reproduce any desired experimental result. This approach works well as long as the design remains within the range of applicability of these parameters. Unfortunately, the range may not be well defined so that if a new gun design is used, or a new propellant or a novel charge configuration is employed the predictions of empirical models cannot be trusted. This observation indicates that all aspects of the physics and chemistry of interior ballistics should be modeled as accurately as possible.

Unfortunately, the ballistic environment is quite hostile, and its detailed study has not been easy. The high pressures and temperatures involved make an experimental approach quite difficult. Some progress has been made, for example, in the application of CARS spectroscopy (ref 1) to propellant combustion but generally progress has been painfully slow. To date no one has devised experiments capable of directly measuring equation of state parameters or transport properties of propellant gases in the ballistic environment. Since good experimental data are not available, the description of unknown properties is either included with the help of adjustable parameters or neglected entirely. It is well understood that since guns operate at high pressure and temperature the ideal gas equation cannot be used. The next best approximation is to use the Abel-Nobel equation of state which includes a covolume term. The general form of this equation is an exact solution to the problem of hard rods moving in one dimension. For two and three dimensions the Abel-Nobel equation is not a good approximation because it does not take into account how hard disks and hard spheres pack together. Real molecules are not hard, but their energy of interaction increases as they come closer together. For this reason the hard sphere diameter should be a function of temperature. At elevated temperatures, more energy is available when molecules collide so that they can come closer together. Finally, real molecules also have an attractive part to the interactive potential otherwise gases would never condense into liquids. At high temperatures the attractive part of the potential makes a small contribution, but it still should be taken into account.

An important contribution to the theory of hot, dense gases was provided by Haar and Shenker (ref 2). These workers approximated the equation of state for a real gas using the second virial coefficient and a closed form expression for all the other virial coefficients using the solution to the hard sphere Percus-Yevick equation. In their equation the hard sphere diameter or "molecular volume" was treated as a parameter and was assumed to be temperature dependent. This approach was developed for H_2O, CO, CO_2, H_2, and N_2 by Powell, Wilmot, Haar and Klein (ref 3). However, these authors did not consider all the minor species which are also present in the propellant gas. Recently, Vladimiroff (ref 4) corrected this defect in the equation of state. For many minor species which are predicted to occur in a propellant gas after combustion, the equation of state parameters are not known. The contributions of all minor species were assumed to be approximated by a Lennard-Jones gas with $\varepsilon/\kappa =$ 100K and $\sigma = 3.0$A. Expressions were developed for the second virial coefficient and the molecular volume and incorporated as a sixth species into the equation of state proposed by Powell, Wilmot, Haar and Klein (ref 3). During the ballistic cycle, conditions inside the gun change. The volume increases, the number of moles of propellant gas changes and the temperature drops because work is being performed on the bullet. In order to calculate the equilibrium composition of the propellant gas as a result of changing conditions inside the gun the thermodynamic code developed by Vladimiroff, Carignan, Chiu and Macpherson (ref 5) was employed. However, all the energy loss terms including work done by the system and heat transferred from the gun are subtracted from the heat of formation of the consumed propellant before the equilibrium calculation is performed. Similar calculations were undertaken for the closed bomb by Robbins and Horst (ref 6) using the BLAKE (ref 7) thermodynamic code.

THE COMPUTER PROGRAM

These considerations were coded in FORTRAN and incorporated into IBHVG2 (interior ballistics of high velocity guns [ref 8]) on an IBM RISC/6000 work station. A real gas equation of state is used as discussed earlier. The conventional calculation using the Abel-Nobel equation of state can be performed as well by setting the parameter OLDWAY = true. The program uses 40 elements and 800 product species. Thermodynamic data from the latest JANNAF tables (ref 9) are employed. A $COMP directive has been added to the standard IBHVG2 (ref 8) input with the propellant composition. The covolume, impetus, flame temperature and gamma are not used but calculated at each time step using an equilibrium assumption. Data on 165 propellant constituents are contained on a file called FUELS. Presently, the program is restricted to 800 product species that are contained on a file called PRODUCTS. The products are those commonly expected with standard propellants which are based on carbon, oxygen, hydrogen, and nitrogen. For special cases, special product files may have to be developed. The output of the program is standard IBHVG2 (ref 8) except the propellant composition is included.

RESULTS AND DISCUSSION

In order to get some feeling for how our equation of state differs from the Abel-Nobel equation the pressure due to the combustion gases produced by M30 propellant was calculated at several temperatures and loading densities and displayed in table 1. It is obvious the Abel-Nobel parameters were fairly well optimized for the conditions inside a gun with errors of the order of 1 or 2 percent. The largest errors are found at 1000K, but this temperature is not encountered in our simulation. Variations in gamma and the moles of gas produced by M30 propellant are reported in table 2 as a function of temperature and loading density. IBHVG2 (ref 8) uses gamma = 1.243 and a gram of M30 propellant is assumed to produce .04215 moles of gas. According to our calculations, gamma is independent of loading density and increases slightly as temperature decreases. If the gamma - 1 approximation is employed differences as high as 15% can be achieved. The moles of gas produced is also found to be independent of loading density but decreases as temperature decreases. This is because at the higher temperatures there is more energy available and there is a greater tendency for molecules to dissociate producing fragments thus increasing the number of moles of gas. The constant value used with the IBHVG2 (ref 8) code seems to be a good average value. Similar calculations are carried out for JA2 propellant and depicted in tables 3 and 4. It might be significant that with the exception of 3500K and a loading density of 0.1 gm/cm^3, the pressure using MCVECE is always lower. The best overall agreement is observed to be at high temperature and for 0.1 to 0.2 loading density.

Interior ballistic calculations using the modified IBHVG2 code were performed next. Three examples were considered based on case 1, case 3, and case 6 in reference 8. Input parameters were left as is except for case 6 where a single charge weight of 17.5 pounds was used and the inner and outer webs were decreased to .07 so that burnout would be achieved inside the gun. The results of our calculations are summarized in tables 4 through 7 and compared with the more conventional approach. The calculations for the HARP gun with M30 propellant and a 52-pound projectile are virtually the same except that Pmax occurs at a slightly earlier time in the conventional calculation. For the M203 charge with the M549 projectile the exit velocities are about the same with both methods. In table 6 it can be seen that the peak pressure occurs about 4.3 ms earlier and is about 7% higher when the old method is employed. The largest differences are observed for the 120-mm system with JA2 propellant and a 15.65-pound projectile. The peak pressure is achieved about 2.5 ms earlier and is about 26% higher with the regular IBHVG2 calculation. The velocity is about 6% lower with the new approach.

CONCLUSIONS

In this work, an attempt was made to solve the energy equation for the ballistic cycle as accurately as possible. The propellant gas is not a monolithic substance which can be described by a simple relationship between the temperature, pressure, and density. In fact, propellant combustion produces molecules and radicals which are then free to interact with each other as conditions inside the gun change. The resulting propellant gas composition was calculated based on an equilibrium assumption. At each step of the ballistic cycle, the heat of formation of the consumed propellant was calculated. The energy losses as computed by the IBHVG2 (ref 8) code and the energy of the products were subtracted from this value and the remaining energy was used to heat up the propellant gas to some temperature. Accurate heat capacities at constant volume from the JANNAF tables (ref 9) were used for all the gas species. The composition and temperature were adjusted until they were self consistent. The pressure was then calculated using the accurate equation of state proposed by Powell, Wilmot, Haar and Klein (ref 3). This pressure was then used in the next step in the ballistic cycle by the IBHVG2 (ref 8) code. All these extra computations do not seem to produce significant differences for the HARP gun and the M203 charge, but they do seem to make a difference for the 120-mm tank gun and JA2 propellant.

At the heart of this calculation is the equilibrium assumption. Since the temperature and density during the ballistic cycle are high, there should be enough energetic collisions between molecules so the thermodynamic and chemical equilibrium will be maintained on a time scale which is short compared to the time step used to integrate the projectile motion. This makes it possible to calculate the composition of the propellant gas by minimizing the free energy. However, if solids or liquids are produced as the propellant gas cools, they may not have time to reach their equilibrium values as assumed in the calculation. It is too early to tell exactly why the two versions of IBHVG2 yield calculated performance which are different for the 120-mm tank gun. One possible explanation is that initially IBHVG2 overestimates the energy available. This is consistent with the observation that for early times IBHVG2 pressures tend to exceed experimental values (ref 8). As can be seen from table 1, subsequent pressures are underestimated for M30 using a covolume equation of state resulting in reasonable agreement between the two methods. On the other hand, for JA2, IBHVG2 overestimates the pressure at later times thus resulting in significant differences for the 120-mm tank gun. At this point a programming error cannot be ruled out, although the work consists of the combination of two working codes with minor scaling and unit conversions required.

Lumped-parameter interior ballistic codes have been used for many years. Comparison with gun firings have yielded a set of assumptions and parameters which work well together. Changing one assumption and eliminating some parameters will not necessarily produce better agreement with experiment unless other parameters and assumptions are changed as well in order to form a self-consistent description of the ballistic event. For example the burning rate for JA2 propellant used in the last example may be consistent with a covolume equation of state but not very consistent with the equation of state used in this work. The significant thing is that an accurate solution of the energy equation does seem to make a difference in some cases. These differences should be investigated further in order to achieve a better understanding of how large caliber guns work.

Table 1. Comparison of Abel-Nobel and MCVECE pressures for M30 propellant

Temperature	Loading density, 0.1 gm/cm^3			Loading density, 0.2 gm/cm^3		
K	Abel-Nobel	MCVECE	% error	Abel-Nobel	MCVECE	% error
3500	19,832	20,465	3.1	44,807	45,960	2.5
3000	16,999	17,449	2.5	38,406	39,258	2.2
2500	14,166	14,487	2.2	32,005	32,592	1.8
2000	11,333	11,523	1.6	25,604	25,853	1.0
1500	8,499	8,519	0.2	19,203	18,724	-2.6
1000	5,666	4,568	-24.0	12,802	9,667	-32.4

	Loading density, 0.3 gm/cm^3			Loading density, 0.4 gm/cm^3		
	Abel-Nobel	MCVECE	% error	Abel-Nobel	MCVECE	% error
3500	77,224	77,839	0.8	120,990	117,748	-2.8
3000	66,192	66,643	0.7	103,706	101,130	-2.5
2500	55,160	55,408	0.4	86,422	84,328	-2.5
2000	44,128	43,936	-0.4	69,137	66,986	-3.2
1500	33,096	31,269	-5.8	51,853	47,027	-10.3
1000	22,064	15,769	-39.9	34,569	23,383	-47.8

Pressures are in the units of psi.

The covolume is 1.02962 cm^3/gram.

Table 2. Gamma and moles of gas from M30 propellant*

Temperature K	Loading density, 0.1 gm/cm³ Gamma	Loading density, 0.1 gm/cm³ Moles of gas	Loading density, 0.2 gm/cm³ Gamma	Loading density, 0.2 gm/cm³ Moles of gas
3500	1.250	.04327	1.249	.04316
3000	1.253	.04310	1.252	.04307
2500	1.257	.04305	1.257	.04303
2000	1.266	.04303	1.266	.04297
1500	1.279	.04255	1.275	.04182
1000	1.264	.03655	1.260	.03615

Temperature K	Loading density, 0.3 gm/cm³ Gamma	Loading density, 0.3 gm/cm³ Moles of gas	Loading density, 0.4 gm/cm³ Gamma	Loading density, 0.4 gm/cm³ Moles of gas
3500	1.248	.04310	1.248	.04307
3000	1.252	.04303	1.251	.04301
2500	1.257	.04299	1.257	.04297
2000	1.265	.04292	1.265	.04286
1500	1.271	.04122	1.268	.04073
1000	1.259	.03697	1.258	.03587

*Calculated using the MCVECE thermodynamic code as a function of temperature and loading density.

The IBHVG2 code uses a gamma = 1.243 and a gram of M30 propellant is assumed to produce .04215 moles of gas.

Table 3. Comparison of Abel-Nobel and MCVECE pressures for JA2 propellant

Temperature	Loading density, 0.1 gm/cm^3			Loading density, 0.2 gm/cm^3		
K	Abel-Nobel	MCVECE	% error	Abel-Nobel	MCVECE	% error
3500	18,936	19,020	0.4	42,563	42,446	-0.3
3000	16,231	16,206	-0.2	36,482	36,228	-0.7
2500	13,526	13,450	-0.6	30,402	30,053	-1.2
2000	10,820	10,696	-1.2	24,322	23,827	-2.1
1500	8,115	7,916	-2.5	18,241	17,293	-5.5
1000	5,410	4,049	-33.6	12,161	8,398	-44.8
	Loading density, 0.3 gm/cm^3			Loading density, 0.4 gm/cm^3		
	Abel-Nobel	MCVECE	% error	Abel-Nobel	MCVECE	% error
3500	72,871	71,434	-2.0	113,162	107,366	-5.4
3000	62,461	61,093	2.2	96,996	92,082	-5.3
2500	52,051	50,736	-2.6	80,830	76,666	-5.4
2000	41,641	40,206	-3.6	64,664	60,861	-6.2
1500	31,231	28,656	-9.0	48,498	42,731	-13.5
1000	20,820	13,416	55.2	32,332	19,370	-66.1

Pressures are in the units of psi. The covolume is 0.9928 cm^3/gram.

Table 4. Gamma and moles of gas from JA2 propellant*

Temperature K	Loading density, 0.1 gm/cm³ Gamma	Loading density, 0.1 gm/cm³ Moles of gas	Loading density, 0.2 gm/cm³ Gamma	Loading density, 0.2 gm/cm³ Moles of gas
3500	1.239	.04045	1.238	.04036
3000	1.241	.04029	1.240	.04026
2500	1.245	.04022	1.245	.04022
2000	1.254	.04022	1.254	.04019
1500	1.266	.03999	1.262	.03925
1000	1.240	.03393	1.236	.03344

Temperature K	Loading density, 0.3 gm/cm³ Gamma	Loading density, 0.3 gm/cm³ Moles of gas	Loading density, 0.4 gm/cm³ Gamma	Loading density, 0.4 gm/cm³ Moles of gas
3500	1.237	.04031	1.237	.04027
3000	1.240	.04024	1.240	.04022
2500	1.245	.04021	1.245	.04019
2000	1.253	.04016	1.253	.04013
1500	1.258	.03868	1.255	.03823
1000	1.234	.03328	1.233	.03317

*Calculated using the MCVECE thermodynamic code as a function of temperature and loading density.

As used in IBHVG2 JA2 gamma = 1.2257 and a gram of JA2 propellant is assumed to produce .04041 moles of gas.

Table 5. Comparison of interior ballistic simulation for HARP gun*

	New		Old	
Conditions at	Pmax	Muzzle	Pmax	Muzzle
Time (ms)	7.30	17.96	7.19	17.94
Travel (in.)	45.87	570.50	44.89	570.50
Velocity (ft/s)	2040.00	5025.00	2059.00	4970.00
Acceleration (G)	22753.00	2385.00	22539.00	2298.00
Breech press (psi)	45549.00	5932.00	45141.00	5756.00
Mean press (psi)	40417.00	5394.00	40057.00	5237.00
Base press (psi)	30153.00	4318.00	29890.00	4200.00
Mean temp (K)	2774.00	1777.00	2743.00	1747.00

*Using IBHVG2 and MCVECE HARP gun with M30 propellant and a 52-pound projectile.

Table 6. Comparison of interior ballistic simulation for the near M203/M549 *

	New		Old	
Conditions at	Pmax	Muzzle	Pmax	Muzzle
Time (ms)	11.00	17.65	6.71	14.11
Travel (in.)	33.84	205.00	20.62	205.00
Velocity (ft/s)	1266.00	2674.00	1029.00	2701.00
Acceleration (G)	10953.00	2659.00	11774.00	2629.00
Breech press (psi)	42459.00	11378.00	45575.00	11284.00
Mean press (psi)	40854.00	10988.00	43831.00	10895.00
Base press (psi)	37645.00	10209.00	40343.00	10116.00
Mean temp (K)	2628.00	1923.00	2699.00	1914.00

*Using IBHVG2 and MCVECE for the near M203/M549 with M30 A1 propellant.

Table 7. Comparison of interior ballistic simulation for the 120-mm tank gun*

	New		Old	
Conditions at	Pmax	Muzzle	Pmax	Muzzle
Time (ms)	6.10	9.10	3.55	6.93
Travel (in.)	43.21	187.11	21.47	187.11
Velocity (ft/s)	2566.00	5015.00	2105.00	5327.00
Acceleration (G)	35171.00	13048.00	47720.00	11999.00
Breech press (psi)	48331.00	18714.00	65404.00	17376.00
Mean press (psi)	42394.00	16417.00	57374.00	15243.00
Base press (psi)	31645.00	12248.00	42809.00	11373.00
Mean temp (K)	2981.00	2387.00	2995.00	2198.00

*Using IBHVG2 and MCVECE for the 120-mm tank gun with JA2 propellant and a 15.65-pound projectile

REFERENCES

1. Harris, L.E. and McIlwain, M.E., Combustion and Flame, 48, 97, 1982.

2. Haar, L. and Shenker, S.H., J. Chem. Phys, 55, 4951, 1971.

3. Powell, E.G., Wilmot, G.B., Haar, L., and Klein, M., "Interior Ballistics of Guns," Krier, H. and Summerfield, M., Editors, Vol 66, Progress in Astronautics and Aeronautics, AIAA, New York, p. 325, 1979.

4. Vladimiroff, T.," Modification of the User Friendly Thermodynamic Code to Include the Effects of Minor Species", 27th JANNAF Combustion Meeting, CPIA Publication 557, Vol I, p. 233, 1990.

5. Vladimiroff, T., Carignan, Y.P., Chiu, D.S., and Macpherson, A.K., "The Development of a User Friendly Thermodynamic Code for the Personal Computer," 24th JANNAF Combustion Meeting, CPIA Publication 476, Vol II, p. 39, 1987.

6. Robbins, F.W., and Horst, A.W., "Numerical Simulation of Closed Bomb Performance Based on Blake Code Thermodynamic Data," IHMR 76-259, Naval Ordnance Station, Indian Head, MD, November 1976.

7. Freedman, E., "BLAKE - A Thermodynamics Code Based on TIGER: User's Guide and Manual," ARBRL-TR-02411, Ballistic Research Laboratory, Aberdeen Proving Ground, MD, July 1982.

8. Anderson, R.D., and Fickie, K.D., "IBHVG2-A User's Guide," BRL-TR-2829, Ballistic Research Laboratory, Aberdeen Proving Ground, MD, July 1987.

9. JANNAF Thermochemical Tables, 3rd Edition, compiled by M.W. Chase (Issued as Supplement No. 1 to Vol 14 (1985) of J. Phys Chem, ref data).

DISTRIBUTION LIST

Commander
Armament Research, Development and Engineering Center
U.S. Army Armament, Munitions and Chemical Command
ATTN: SMCAR-IMI-I (3)
SMCAR-AEE (3)
SMCAR-AEE-B (5)
Picatinny Arsenal, NJ 07806-5000

Commander
U.S. Army Armament, Munitions and Chemical Command
ATTN: AMSMC-GCL (D)
Picatinny Arsenal, NJ 07806-5000

Administrator
Defense Technical Information Center
ATTN: Accessions Division (12)
Cameron Station
Alexandria, VA 22304-6145

Director
U.S. Army Material Systems Analysis Activity
ATTN: AMXSY-MP
Aberdeen Proving Ground, MD 21005-5066

Commander
Chemical Research, Development and Engineering Center
U.S. Army Armament, Munitions and Chemical Command
ATTN: SMCCR-MSI
Aberdeen Proving Ground, MD 21010-5423

Commander
U.S. Army Edgewood Research, Development and Engineering Center
ATTN: SCBRD-RTT (Aerodynamics Technical Team)
Aberdeen Proving Ground, MD 21010-5423

Director
Army Research Laboratory
ATTN: AMSRL-WT-D
Aberdeen Proving Ground, MD 21005-5066

Chief
Benet Weapons Laboratory, CCAC
Armament Research, Development and Engineering Center
U.S. Army Armament, Munitions and Chemical Command
ATTN: SMCAR-CCB-TL
Watervliet, NY 12189-5000

Commander
U.S. Army Rock Island Arsenal
ATTN: SMCRI-IMC-RT/Technical Library
Rock Island, IL 61299-5000

Director
U.S. Army TRADOC Analysis Command
ATTN: ATRC-WSS-R
White Sands Missile Range, NM 88002